Robustness of s-wave pairing symmetry in iron-based superconductors and its implications to fundamentals on magnetically-driven high temperature superconductivity

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Under the assumption that the superconducting state belongs to a single irreducible representation of lattice symmetry, we argue that the pairing symmetry in all measured iron-based superconductors is universally consistent with the A_{1g} s-wave. The robust s-wave pairing throughout the different families of iron-based superconductors at different doping regions signals two fundamental principles behind high T_c superconducting mechanisms: (1) the correspondence principle: the short range magnetic exchange interactions and the Fermi surfaces act collaboratively to achieve high T_c superconductivity and determine pairing symmetries; (2) the magnetic selection pairing rule: the superconductivity is only induced by the magnetic exchange couplings from the superexchange mechanism through cation-anion-cation chemical bondings. These principles explain why the unconventional high T_c superconductivity appears to be such a rare but robust phenomena with its strict requirement on electronic environment: it can only be achieved on pure bands formed by the cation's d-orbital that have strongly in-plane chemical bonding with anions. The mixture of any other orbitals or destroying superexchange rapidly suppresses superconductivity. The robust s-wave pairing also reveals that the current standard effective models with only onsite interactions are not sufficient and a minimum microscopic model must include strong nearest neighbor repulsive interactions resulted from the d-d direct bondings to serves as a s-wave symmetry stabilizer. Finally, the sign distribution of the superconducting order parameters in the reciprocal space is simply a consequence of the form factors given by the leading short-range pairings. The sign change of superconducting order parameters on Fermi surfaces is not a necessary requirement in repulsive-interaction-driven high T_c mechanism. The results will guide us to search for new electronic structure that supports high T_c superconductivity.

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I. INTRODUCTION

The discovery of iron-based superconductors[1] six years ago dethroned the cuprates as the dictator of high T_c superconductors in correlated electron systems and generated great hope and excitement to solve the decades-odd problem of non-BCS (Bardeen, Cooper and Schrieffer) high T_c mechanism. There were fundamental reasons for such an optimistic hope. Iron-based superconductors were quickly revealed[2–4] to share many common electronic properties with the cuprates, including a close proximity to an antiferromagnetic (AFM) order phase[5]. The similarity between the two superconductors strongly suggests that there should be one unified high T_c superconductivity mechanism. In the meantime, iron-based superconductors exhibit many distinct physical properties from the cuprates. The differences between these two materials also provide us an opportunity to determine side effects that are irrelevant to the superconducting mechanism.

However, the optimism was dying out in the past several years as more iron-based superconductors[3, 4] were discovered and an unified understanding of all materials became increasingly difficult. In particular, pairing symmetries in iron-based superconductors have recently become more controversial than ever before[6]. A variety of new possible pairing symmetries were proposed and many theories suggested that there is no universal pairing symmetry among iron-based superconductors[6–8]. Namely, pairing symmetries are material and doping dependent. This situation is very similar to the research status of the cuprates in the early 90's before the d-wave pairing symmetry was finalized[9]. The d-wave pairing symmetry in the cuprates is widely acknowledged as the major evidence to distinguish the cuprates from conventional BCS-type s-wave superconductors. The robustness of the d-wave pairing in the cuprates is one of the main supports for magnetically-driven high T_c superconducting mechanisms[10, 11]. Thus, without a consensus on the pairing symmetry in iron-based superconductors, it is difficult to imagine that the study of iron-based superconductors can help to advance the understanding of high T_c superconducting mechanisms.

The pairing symmetry controversy in iron-based superconductors were largely caused by the "top-to-bottom" theoretical studies. The study of correlated electron materials or materials that are believed to be in that category has been customized to

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standardized models and methods[10, 11], inherited from the past intensive research in cuprates. After iron-based superconductors were discovered, the extended versions of these standardized models, such as Hubbard-type[6] or 't-J' -type models[12–14], were immediately deployed. The pairing symmetries in iron-based superconductors were analyzed with a variety of methods[6]. The theoretical predictions on the pairing symmetries are in turmoil[6]. In particular, as Fermi surfaces in iron-based superconductors can vary significantly in different doping regions, as well as in different families of iron-based superconductors, standard theoretical methods, due to their high sensitivity to the change of Fermi surfaces, suggest that the pairing symmetries would vary significantly as well.

However, if we take the "bottom-up" approach and examine the experimental evidence for the pairing symmetries in iron-based superconductors, it is remarkable that all experimental investigations that directly probe the superconducting pairing symmetry point to an universal s-wave pairing symmetry in all measured materials[15], including the recent discovered materials[16–18]. Thus, the robust s-wave pairing symmetry in iron-based superconductors is not only a challenge but also offers an opportunity to establish fundamentals in magnetically-driven high T_c superconducting mechanisms.

II. PAIRING SYMMETRIES AND GAP FUNCTIONS

Before we discuss the experimental evidence, for the sake of clarification, a few acceptable assumptions and notations should be addressed. First, we focus on uniform superconducting state. Namely, the state has the original lattice translational symmetry. Second, we assume that the pairing in iron-based superconductors is spin-singlet. This assumption has been supported by many experiments throughout different families of iron-based superconductors[3, 4, 6]. Third, we make clear that throughout the paper, unless it is otherwise specifically stated, we use the $1-Fe$ unit cell to label momentum space[19]. In this case, because the natural unit cell for iron-based superconductors is a $2-Fe$ unit cell, in the 11 ($FeSe$), 111 ($NaFeAs$) or 1111 ($LaOFeAs$) types of materials that have non-symmorphic space group $P4/nmm$ and the 122 ($BaFe_2As_2$) type of materials that has space group $I4/mmm$, the $\vec{Q}_1=(\pi,\pi,0)$ and $\vec{Q}_2=(\pi,\pi,\pi)$ in the reciprocal lattice of the $1-Fe$ unit cell are reciprocal lattice vectors in the original $2-Fe$ unit cell[7]. In the following part of paper, as we primarily focus on the two dimensional electronic structures of the building block, the $FeAs/Se$ layer, which is equivalent to setting $k_z=0$ for the bulk materials, both $\vec{Q}_1$ and $\vec{Q}_2$ are reduced to $\vec{Q}=(\pi,\pi)$. Finally, as pointed out in Ref.[7], there are two types of pairing that do not break translational symmetries with respect to the $2-Fe$ unit cell in iron-based superconductors, the normal pairing which is between two particles with opposite momentums, namely, $(\vec{k},-\vec{k})$ and the η pairing which is specified by corresponding paired momentums, as $(\vec{k},-\vec{k}+\vec{Q})$. The difference between these two types of pairings are classified by the parity difference with respect to the center on the nearest neighbour (NN) $Fe-Fe$ bonds. Because of this difference, the mixture of normal and η pairing is also not a pure state. Since a pure η pairing is almost impossible under reasonable conditions, we will ignore the η pairing in the following as well.

Assuming the superconducting state is a pure state, the pairing symmetry is manifestly reflected in superconducting gap functions in the reciprocal space. For iron-based superconductors, if we take $k_z=0$ and ignore spin-orbital couplings, which is known to be small[20], the normal pairing can be classified by the D_{4h} group, which is the same as cuprates. Except the A_{1g} s-wave, all other pairing symmetries have fixed gapless nodes along some high symmetry lines in the reciprocal space. In Fig.1, we draw four typical Fermi surface topologies. The Fig.1(a) represents heavily hole doped iron-pnictides such as KFe_2As_2. There are three hole pockets at the zone center (Γ) and four small hole pockets at the zone corner (M). With increasing electron doping, the four hole pockets at the zone corner become two electron pockets as shown in Fig.1(b) which represents the typical Fermi surfaces in iron-pnicitides within large doping regions. It is also important to note that depending on the doping and materials, the number of hole pockets at the zone center as shown in Fig.1(a,b) can also vary. For example, in the bulk $FeSe_xTe_{1-x}$ materials[15], there are only two hole pockets at the zone center and in the heavily electron doped $LiFeAs$[15], there could be just one hole pocket at the zone center. With further increasing electron doping, the hole pockets at the zone center can be suppressed completely as shown in the Fig.1 (c). The heavily electron doped iron-pnictides and many iron-chalcogenides, including the superconducting KFe_2Se_2[21], the superconducting single layer $FeSe$ grown on the $SrTiO_3$ substrate[22–24] and $(Li,Fe)OHFeSe$[16–18], have such a typical Fermi surface topology. Away from the $k_z=0$ plane, heavily electron doped KFe_2Se_2 can also have a small three dimensional electron pocket as shown in Fig.1(d) where a small electron pocket appears at the zone center at $k_z=\pi$[25].

In the presence of the hole pockets at the zone center as shown in Fig.1(a,b), a direct measurement of the gap functions on the hole pockets can determine the pairing symmetry. The angle resolved photoemission spectroscopy (ARPES) has measured a variety of iron-based superconductors[15, 26] that exhibit hole pockets at the zone center, including hole doped $Ba_{2-x}K_xFe_2As_2$, electron doped $Li(Na)Fe_{1-x}CoAs$, isovalent doped $BaFe_2(As_{1-x}P_x)_2$ and $BaFe_{2-x}Ru_xAs_2$, and $FeSe_{1-x}Te_x$. There are two common results on the measured gap functions of the hole pockets. *First, the inner smallest hole pocket always has the largest full superconducting gap that is close to be isotropic. Second, the superconducting gap sizes on the hole pockets generally follow the rule: larger gaps on smaller hole pockets[15].* These two facts are valid in all measured doping regions. If the superconducting state is a pure state, the two common results are only consistent with the s-wave pairing. In fact, even if we

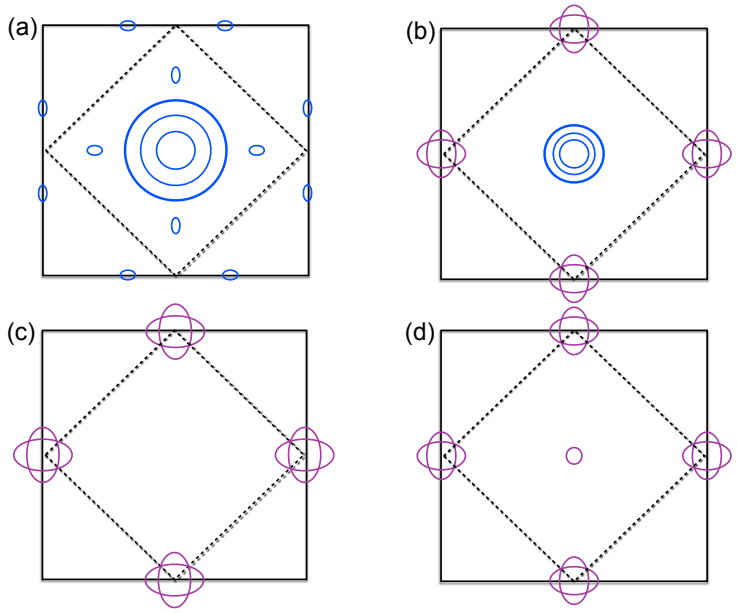

FIG. 1: The typical Fermi surface topologies of iron-based superconductors: (a) Heavily hole doped (KFe_2As_2); (b) Near optimally doped iron-pnictides; (c) Heavily electron doped (single layer $FeSe/STO$, $(Li,Fe)OHFeSe$ and KFe_2Se_2 at $k_z = 0$) ; (d) KFe_2Se_2 at $k_z = \pi$.

do not assume a pure state, these results suggest that the s-wave pairing must be the dominant component.

In the case shown in Fig.1(c,d), in which there is no hole pockets at the zone center, a full gap structure on the electron pockets[16–18, 21] was also universally observed. This full gap structure is generally only consistent with the s-wave pairing symmetry. For a bulk material, the nodes on electron pockets are inevitable if it is a d-wave pairing state[27]. In the case of Fig.1(d), which represents the Fermi surfaces of KFe_2Se_2 at $k_z = \pi$, there is another direct evidence for the s-wave pairing symmetry: the small electron pocket at the zone center has almost isotropic full gap[21, 25]. A case that needs to be specifically addressed is the single layer $FeSe/STO$[22–24]. In this case, a full gap structure on electron pockets, in principle, can be consistent with the B_{1g} d-wave. However, if we consider the hybridization between two electron pockets at the zone corner caused by the spin-orbital couplings and the lattice symmetry breaking induced by the substrate, gapless nodes must generally appear in the B_{1g} d-wave state. Therefore, a full gap structure on electron pockets is also only consistent with a s-wave state.

Besides the direct gap function measurements of ARPES, the scanning tunneling microscopy(STM) also reveals full gap structure in many different materials[3]. The measurements on tunneling junctions also support the s-wave pairing symmetry[2].

It is also important to mention that there is indirect evidence to support the d-wave pairing in some materials of iron-based superconductors. For example, possible d-wave pairing symmetry is indirectly indicated in KFe_2As_2 by thermal conductivity measurements and pressure effect[28]. However, this indirect indication is not conclusive. The thermal transport probes the existence of low energy excitations, namely, the existence of superconducting nodes on Fermi surfaces. But it does not specify the structure of the nodes. In fact, the ARPES measurements in KFe_2As_2 have shown that there are possible gapless nodes in the outer hole pockets[29, 30] but the inner hole pocket is fully gapped. Nodes have also been directly observed by ARPES in $BaFe_2(As_{1-x}P_x)_2$ in the outer hole pocket at the zone center[31]. Thus, the development of the accidental nodes appears to be tied with the enlargement of the outer hole pockets in both KFe_2As_2 and $BaFe_2(As_{1-x}P_x)_2$[32], in which the pockets reach close to the middle point of the first Brillouin zone.

In summary, the full gap structure on Fermi pockets observed in a variety of iron-based superconductors at different doping regions is only consistent with the A_{1g} s-wave pairing symmetry. The appearance of the largest isotropic gap on the smallest hole pocket suggests that the s-wave component dominates even if the superconducting state is not a pure state.

III. THEORETICAL RESULTS ON PAIRING SYMMETRIES OF IRON-BASED SUPERCONDUCTORS

Through intensive research in cuprates, we have been accustomed to use two types of standard models to investigate correlated electron systems. The first type of standard models includes the band structure near Fermi surfaces and effective local repulsive interactions in the spirit of the Hubbard model. The second type of standard models includes an effective band structure and effective short-range magnetic exchange couplings in the spirit of the 't-J' model. In cuprates, the d-wave pairing symmetry is

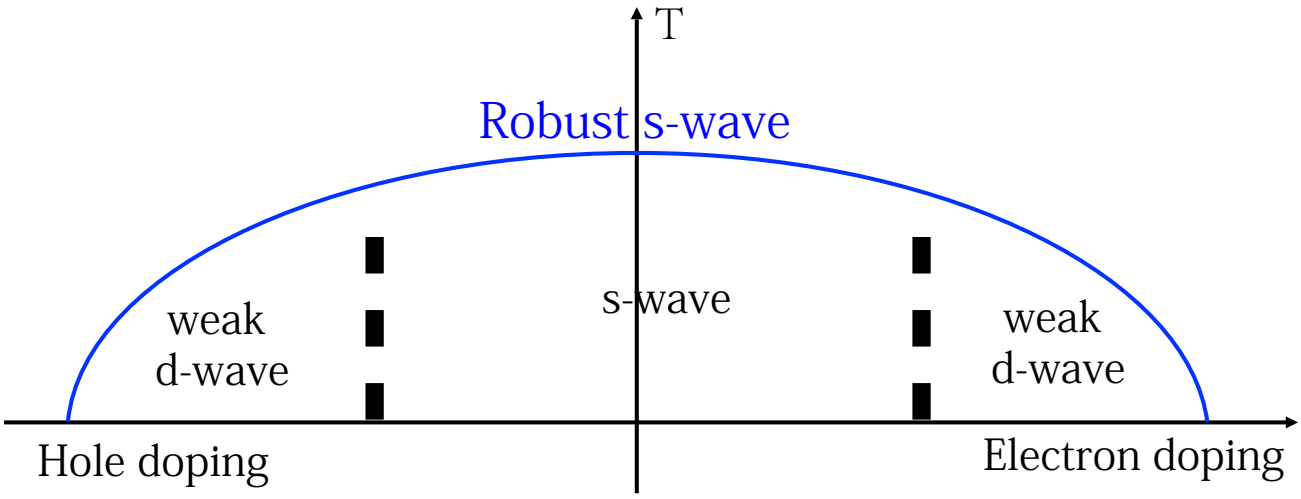

FIG. 2: The sketch of controversial pictures on pairing symmetries of iron-based superconductors as a function of doping: a robust s-wave pairing symmetry vs theoretical results as indicated by the black text) from the $t-U-J_H$ model in Eq.2.

obtained consistently in both types of models[33–37]. In fact, it is well-known that two models in cuprates are intimately linked. There are also reasonable microscopic derivations to support them in capturing essential physics of cuprates[38].

However, for iron-based superconductors the situation is rather different. The first type of models in iron-based superconductors is generally proposed as[6]

$$\hat{H}_U = \hat{H}_0 + \hat{H}_I, \tag{1}$$

$$\hat{H}_I = \sum_i [\sum_{a\neq b} (J_H \hat{S}_{ai}\cdot\hat{S}_{bi} + U'\hat{n}_{ai\uparrow}\hat{n}_{bi\downarrow}) + U\hat{n}_{ai\uparrow}\hat{n}_{ai\downarrow}], \tag{2}$$

where $\hat{H}_0$ describes the effective multi-orbital band structures based on the five d orbitals of irons[39], a, b label orbitals and i labels the sites of the iron square lattice. The interactions include all onsite interactions including the Hund's coupling J_H, intra-orbital repulsive interaction U and inter-orbital repulsive interaction U'. Considering the interactions in the weak to intermediate regions, the model has been treated by a variety of approximate methods including random phase approximation(RPA)[6], perturbative renormalization analysis[40] and numerical functional renormalization analysis (FRG)[41]. The pairing symmetries obtained from the model depend on the detailed structures of Fermi surfaces. In general, the strongest superconductivity is achieved when hole pockets and electron pockets are close to the nesting condition. In this case, the pairing symmetry is the s-wave pairing symmetry, called $s_{\pm}$, which is characterized by the sign change of the superconducting order parameters between the hole and electron pockets in momentum space. With increasing hole (or electron) doping, the large anisotropic gap is expected to be developed on hole (or electron) pockets and a transition from the s-wave to d-wave pairing symmetry is expected[42, 43]. In the Fig.2, we sketch the phase diagram for the pairing symmetries from these theoretical studies. Corresponding to the Fermi surfaces shown in Fig.1, the results suggest the d-wave pairing for Fig.1(a,c,d) and the s-wave for Fig.1(b).

A strong message from the above theoretical studies is that there is no universal pairing symmetry in iron-based superconductors. This conclusion is in direct conflict with the experimental observations. Moreover, within these studies, the strongest superconductivity is obtained when hole and electron pockets both exist and are close to the nesting conditions. The theory clearly fails to explain the existence of the high T_c superconductivity at heavily electron doped region of many $FeSe$-based compounds.

In the second type of models, the starting Hamiltonian[13] is

$$\hat{H}_{tJ} = \hat{\tilde{H}}_0 + \hat{H}_J, \tag{3}$$

$$\hat{H}_J = \sum_{ij} J_{ij}\hat{S}_i\cdot\hat{S}_j, \tag{4}$$

$$\tag{5}$$

where $\hat{\tilde{H}}_0$ describes the renormalized effective band structure and $\hat{H}_J$ describes the effective magnetic exchange couplings. The pairing symmetry has been studied by including both NN magnetic exchange couplings, $J_{<ij>} = J_1$ and next nearest neighbour (NNN) ones, $J_{<<ij>>} = J_2$. Namely, H_J becomes

$$\hat{H}_J = \sum_{<ij>} J_1 \hat{S}_i \cdot \hat{S}_j + \sum_{<<ij>>} J_2 \hat{S}_i \cdot \hat{S}_j. \tag{6}$$

Within this model, a robust s-wave pairing symmetry can be achieved if the NNN AFM exchange coupling J_2 dominates regardless of the presence or absence of the hole pockets[14]. However, if the NN AFM exchange couplings are significant, the pairing symmetry is also expected to deviate from the s-wave[13].

The pairing symmetry in this model is simply determined by the *'correspondence principle'* between Fermi surface topologies in reciprocal space and the symmetry form factors of short-range magnetic exchange couplings, which we refer it as *the HDLD principle* since it has been specified explicitly by Hu-Ding[44] and Lee-Davis[45] recently. The principle can be applied to unify the understanding of pairing symmetries in both cuprates and iron-based superconductors. In cuprates, the magnetic exchange coupling is dominated by the NN J_1. The d-wave form factor associated with J_1 in the pairing channel is given by $cosk_x - cosk_y$, which can open much larger superconducting gaps than the s-wave form factor $cosk_x + cosk_y$ on the Fermi surfaces of cuprates. In iron-based superconductors, the intra-orbital pairing form factor associated with J_2 in the d-wave symmetry is $sink_x sink_y$, which has much smaller values on Fermi surfaces than the s-wave form factor $cosk_x cosk_y$. Thus, if J_2 is the dominating magnetic exchange coupling, the strong s-wave superconductivity can be achieved in both Fermi surface topologies shown in Fig.1(b,c). However, it is clear that if J_1 is also important, the d-wave form factor $cosk_x - cosk_y$ associated with J_1 can also be very competitive when the electron pockets at the zone corner dominate. In Ref.[14], it is argued that J_1 is inactive in spin-singlet pairing channel in iron-chalcogenides because J_1 based on neutron scattering experimental data is ferromagnetic (FM) so that the s-wave pairing prevails in all iron-chalcogenides[5, 46].

In summary, the first type of the model, $\hat{H}_U$, does not support a robust s-wave. In the second type of model, $\hat{H}_{tJ}$, it requires the dominance of J_2 over J_1 to establish a robust s-wave. However, the assumption of the dominance in the second type of models is not well justified for iron-pnictides where the J_1 value obtained from neutron scattering experiments can be strongly AFM. Therefore, the robust s-wave symmetry in iron-based superconductors exposes serious limitation and deficiency in current standard models based on repulsive interaction (or magnetically) driven superconducting mechanisms.

IV. THE MINIMUM MICROSCOPIC MODELS TO STABILIZE S-WAVE PAIRING IN IRON-BASED SUPERCONDUCTORS

What are the deficiencies in the standard models for iron-based superconductors and how can they be fixed? In the above section, we already notice that the robust s-wave can be obtained from the J_2 AFM exchange. This provides an important clue. In fact, if we carefully check the electronic structure of iron-based superconductors, it is easy to see that J_1 and J_2 involve different microscopic origins.

First, the difference is already implied in the low energy effective model that describes the magnetism in iron-based superconductors. Extracted from neutron scattering experimental data, the value of J_2 is quite universal throughout different families of iron-based superconductors[5, 46]. However it is not the case for J_1. It has shown that the magnetism in iron-based superconductors can be unified by the following effective Hamiltonian,

$$\begin{aligned} \hat{H}_{JK} = & \sum_{<ij>} (J_1 \hat{S}_i \cdot \hat{S}_j - K(\hat{S}_i \cdot \hat{S}_j)^2) \\ + & \sum_{<<ij>>} J_2 \hat{S}_i \cdot \hat{S}_j + \sum_{<ij>TNN} J_3 \hat{S}_i \cdot \hat{S}_j. \end{aligned} \tag{7}$$

This model was proposed as the minimum magnetic model to unify the magnetism in iron-based superconductors[46]. Besides the J_1 and J_2 terms, the model includes the quadruple spin interaction K term between two NN sites and the third NN (TNN) magnetic exchange coupling J_3[47]. The K term was first proposed in Ref.[48] to explain the large anisotropy of the effective NN couplings along two different directions in the collinear AFM order state in iron-pnictides.

There are several important observations related to $\hat{H}_{JK}$: (a) the classical phase diagram of the model[46, 49] includes all observed magnetic long range orders, including both commensurate and incommensurate orders in different families of iron-based superconductors; (b) J_2 in all iron-based superconductors are universally AFM with a similar value while J_1 is not. In iron-pnictides, J_1 is AFM. But in iron-chalcogendies, it changes to FM; (c) the model can even describe the observed magnetic orders in the vacancy ordered states in $K_x Fe_{2-y} Se_2$; (d) J_3 is significant in iron-chalcogenides but small in iron-pnicitides; (e) the K term is significant on the NN bonds. The existence of the quadruple term on the NN bonds and the non-universality of the J_1 value suggest that the mechanisms behind J_1 and J_2 are very different.

Second, there is a major difference between the electronic structures of iron-based superconductors and those of cuprates. In cuprates, without oxygen atoms, the d-orbital of Cu atoms can be treated as localized d-orbital (mootness). The kinetic energy, namely, the effective hopping between two d-orbital is caused by the d-p hybridization. This hybridization simultaneously generates the magnetic superexchange couplings between two NN Cu sites. Therefore, the magnetism involves a pure superexchange mechanism. If we consider an effective model based on the Cu lattice, the Hubbard term is sufficient to capture the superexchange coupling. Therefore, magnetism and superconducting pairing symmetry can be consistently obtained in both 't-J' and Hubbard models. However, in iron-based superconductors, if we remove the As/Se atoms in the $FeAs/Se$ layer and check the iron lattice, the distance between two NN irons is very short. In fact, the distance is very close to the lattice constant in a three dimensional body centered iron metal. Therefore, without As/Se atoms, the large hopping between two NN Fe atoms exists and the iron lattice itself is a metallic state. The chemical bonding between two NN Fe atoms can not be ignored. The difference leads to several important consequences: (1) the hopping through the d-p hybridization that provides the superexchange mechanism is not the hopping defined in the effective Hubbard-type model given in Eq.2; (2) the NN hybridization between the d-orbital can also cause magnetism through direct exchange mechanism; (3) the overlap between two NN d-orbital also suggests that strong repulsive interactions between two NN sites have to be included. Thus, a model with only onsite repulsive interactions is not sufficient to capture the electronic physics of iron-based superconductors. In an effective model with only onsite repulsive interactions given in Eq.2, J_1 and J_2 are both the leading magnetic coupling terms and are developed with equal footing. Thus, the different magnetic origins between J_1 and J_2 are not taken into account by Eq.2.

The above analysis suggests that with only the simple onsite repulsive interaction, $\hat{H}_U$ in Eq.2 is not sufficient to describe iron-based superconductors. If we consider superconducting pairing driven by repulsive interactions, the onsite repulsive interactions only forbid onsite pairings. Without considering the NN repulsive interactions, the NN pairings generally become the leading contribution to pairing gap functions. In the model given by Eq.2, as both NN hoppings and NNN hoppings are large, J_1 and J_2 develop with equal footing as the leading magnetic couplings to provide attractive pairing forces. Because of their competition, the pairing symmetry obtained from Eq.2 is highly sensitive to the change of Fermi surfaces.

The above analysis also provide the solution to fix the problem. The existence of chemical bonding between two NN Fe d orbitals suggests that significant repulsive interactions between the NN sites must exist in the iron-based superconductors. This repulsive interaction can suppress the attractive interactions generated by the onsite interactions. With both repulsive interactions on onsite and between two NN sites, the leading attractive forces must start between the NNN sites so that the robust s-wave can be obtained. Thus, a minimum term that can be added to the Hubbard-type in Eq.2 is

$$\hat{H}_V = \sum_{<ij>,ab} V_{ab}\hat{n}_{ia}\hat{n}_{jb}, \tag{8}$$

where V_{ab} represents the repulsive interactions between two NN sites.

Here, we are not interested in the detailed values of the NN repulsive interaction. Qualitatively, we can argue that this repulsive interaction can serve a s-wave stabilizer. The effect of this term on pairing can be understood in both real and momentum spaces. In the real space, as repulsive interactions exist both on onsite and between NN sites, the attractive force generated for pairing falls to the NNN and the TNN bonds. Namely, the dominated pairing in iron-lattice falls to pairing within each sublattice if we divide the iron lattice to two sublattice A and B. The intersublattice pairing is suppressed. In the reciprocal space, the $\hat{H}_V$ allows two Cooper pairs with pairing momentum $(\vec{k}, -\vec{k})$ and $(\vec{k}+\vec{Q}, -\vec{k}+\vec{Q})$ to be attractive. Therefore, the s_{++} pairing can be robust in presence of only electron pockets at two M points.

To show that $\hat{H}_V$ can serve as a s-wave stabilizer even in a weak coupling approach, we performed a FRG calculation in a parameter region that s-wave and d-wave pairing symmetries are very competitive to each other. We take the band parameters provided by Ref.[39]. This five-band tight-binding model gives five Fermi surfaces when the chemical potential $\mu = -0.17$. In our calculation we set the interaction parameters as $U = 4, U' = 4$. The FRG flow demonstrates that s-wave and d-wave instabilities have approximately the same divergence as the momentum cutoff Λ decreasing(see Fig.3(a)). After adding the NN repulsive interaction V into the interaction part, we obtain a significant enhancement of s-wave instability which indicates $\hat{H}_V$ tents to induce s-wave pairing symmetry. Fig.3(b) shows the FRG flow when $V_{ab} = V = 1.2$ for any a and b, from it we can see that s-wave is distinctly stronger than d-wave.

V. THE EMERGENCE OF THE MAGNETIC SELECTION PAIRING RULE AND FUNDAMENTALS ON ELECTRONIC STRUCTURES FOR HIGH T_c MATERIALS

Unconventional high T_c superconductivity appears to be a rare phenomena. Only two classes of materials were discovered accidentally by intensive researches in the past several decades. However, once it happens, the superconductivity is very robust. These rareness and robustness have already spoken a fundamental difference between unconventional high T_c superconductors and conventional BCS superconductors which can almost ubiquitously take place in most metallic systems at low temperature. The fundamental difference, as many of us believe today, is that the unconventional high T_c superconductors belong to a new

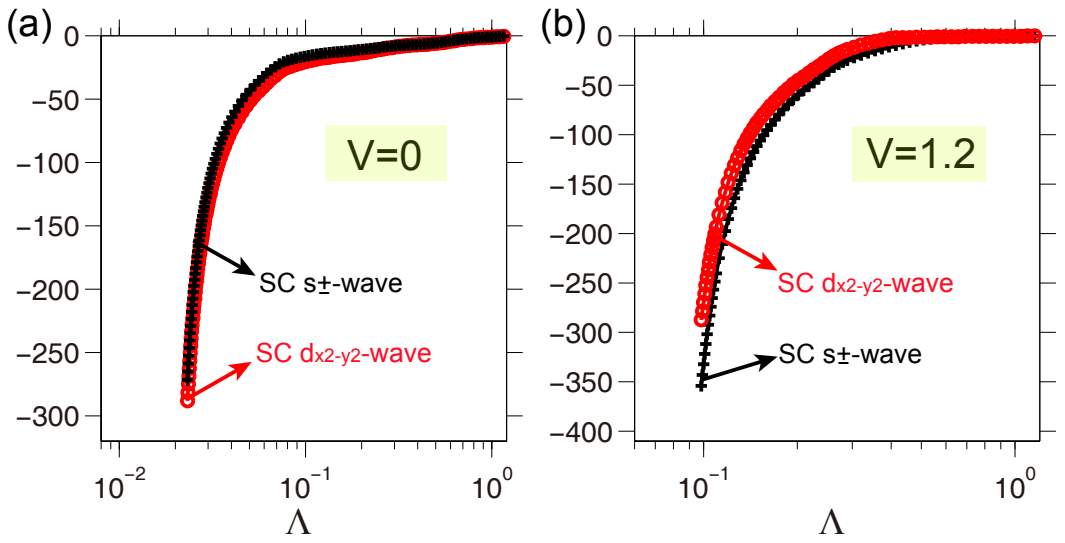

FIG. 3: The FRG flow of superconductivity s-wave and d-wave instabilities for five-band tight-binding model[39] with onsite repulsive interaction U, U' and NN repulsive interaction V: (a) $U = 4, U' = 4, V = 0$, s-wave and d-wave symmetries are very competitive to each other. (b) $U = 4, U' = 4, V = 1.2$, the divergence of s-wave is stronger than d-wave after add V.

material category–correlated electron systems. Nevertheless, even if the materials are in a different category, explaining the rareness and robustness of high T_c phenomena is still a fundamental problem as so many correlated electron systems have been discovered. Theoretically, we have been accustomed to simplify correlation physics into an onsite Hubbard interaction and have used it everywhere. If such a simplified model is applicable to all correlated materials, it is difficult to understand the rareness of high T_c phenomena.

Combining the rareness dillemma, the robustness of pairing symmetries in both high T_c superconductors, the above analysis regarding the origin of the robust s-wave pairing symmetry in iron-based superconductors, we can only think of one logistic answer, that is, *high T_c superconductivity takes place in an electronic environment in which the paired electrons must participate strongly in magnetic superexchange mechanisms. Namely, only magnetic superexchange mechanism drives superconducting pairing.* With this hidden principle, we can understand the rareness problem. Both the d^9 filling configuration in Cu^{2+} in cuprates and the d^6 filling configuration of Fe^{2+} in iron-based superconductors are the unique configurations to make the orbital characters on the Fermi surfaces belong to the orbitals with strong involvement in superexchange processes. Replacing Cu in cuprates or Fe in iron-based superconductors both violate this principle, which explain why the Mn, Co and Ni-based pnicitides are not high T_c superconductors[50–52]. The principle also suggests that the effective standardized Hubbard and 't-J' models are only good approximations if all effective hopping parameters in the models stem from the d-p hybridizations. In fact, the presence of strong correlation effect is generally correlated together with the existence of the superexchange processes.

The above magnetic selection pairing rule, together with the HDDL principle, provides an powerful guide to search for new unconventional high T_c superconductors. The rules are not easy to be satisfied in a three dimensional electronic structure. Here, we focus on materials with a quasi-two dimensional layer structure constructed by transition metal cation-anion complexes. To be a high T_c candidates, the following conditions must be followed:

- *The orbitals (the d-orbital of cations) responsible for high T_c on Fermi surfaces must be strongly coupled to in-plane anions.* This rule follows the fact that the superexchange is meditated through the anions.The stronger coupling can produce stronger superexchange couplings, thus possible stronger superconductivity. In cuprates, the E_g orbital, $d_{x^2-y^2}$, strongly couples to the p-orbital of in-plane oxygen. In iron-based superconductors, it is the three t_{2g} orbitals which strongly couple to the p-orbital of As/Se.

- *The orbitals (the d-orbital of cations) responsible for high T_c on Fermi surfaces should be relatively higher energy orbitals in local crystal field splitting environments.* This rule follows that the orbitals that strongly couple to anions experience a larger crystal field energy. This rule, thus, also implies that cation atoms should have high filling in their d-orbital shells in order to achieve possible high T_c. Namely, the second half transition metal cation atoms, which include both Fe and Cu atoms, are more likely to form potential high temperature superconductors. Of course, this rule does not completely rule out the possibility to achieve high T_c for the first half transition metal cation atoms.

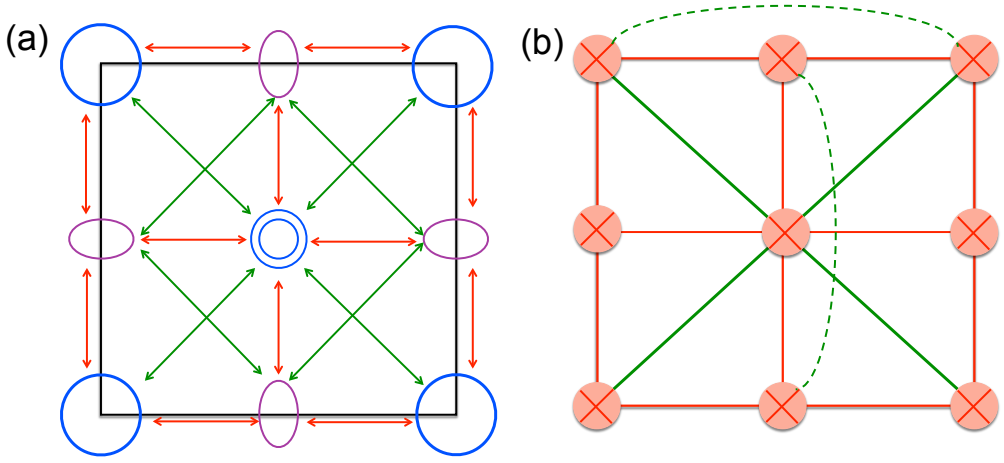

FIG. 4: (a) The pairing interactions between different pockets in the 1-Fe unit cell Brillouin zone for iron-based superconductors (the red and green arrows indicate repulsive and attractive pairing interactions respectively. (b) The real space pairing configurations in the Fe lattice for iron-based superconductors (only the two sites linked by the green lines are allowed to be paired.)

- *There should be no chemical bonding between anions.* The chemical bonding between anions can generally push the anti-bonding states to higher energy which can strongly suppress the superexchange processes. This is the essential reason why the superconductivity and magnetism suddenly disappears in the collapsed $CaFe_2As_2$ phase where the chemical bondings between two As atoms on neighbor layers are formed[53].
- *The weight of other d-orbital on Fermi surfaces, which do not or only weakly couple to in-plane anions, should be as small as possible.* The mixture of the other d-orbital can strongly suppress superconductivity. This fact has been known in cuprates that raising the energy level of the d_{z^2} orbital which increases its' presence near Fermi surfaces strongly suppresses high T_c[54].

In general, the above rules suggest that the electronic environment to host high T_c superconductivity must include quasi-two dimensional bands formed dominantly by the d-orbital through d-p couplings.

VI. SUMMARY AND DISCUSSION

In summary, the robustness of s-wave pairing in iron-based superconductors can only be understood by assuming that the pairing is exclusively formed through the superexhange process. Namely, the superexchange AFM exchange couplings are responsible for superconducting pairing. While this physics is very clear in cuprates, it is not obvious in iron-based superconductors because of the existence of the direct d-d bonding between two NN Fe atoms.

Realizing the origin of pairing from exclusive superexchange AFM has an important impact on search new high T_c materials and understand pairing properties. First, we should target to design or find a pure electronic lattice structure which host bands with dominant contribution from d-orbital that involve strong in-plane d-p hybridization. Second, the superconducting pairing can be better understood in real space than in momentum space as the superexchange process is a local process. Fig.4(a,b) sketches the leading pairing bonds for iron-based superconductors in real space and its corresponding pairing interaction picture in momentum space. A natural consequence of the real space picture is that the sign change of the superconducting order parameters on Fermi surfaces is not a necessary requirement. This implication also suggests that the earlier argument in the weak coupling approach about the $s_{\pm}$ pairing symmetry that is based on momentum space is not completely correct[55]. Third, it is easy to understand why the superconductivity is so robust but in the meanwhile is so sensitive to the lattice parameter change of the anions as the anions essentially mediates superconducting pairing. For example, the $Fe-As-Fe$ angle is a critical parameter in determining T_c in iron based superconductors[3]. Finally, the principles also provide an intuitive explanation about why high T_c superconductivity is absent in many materials with strong magnetic fluctuations.

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